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Andreev Bound-states of vortices and surfaces in topological superconductors

Yuki Nagai, Hiroki Nakamura and Masahiko Machida
CCSE, Japan Atomic Energy Agency, 5-1-5 Kashiwanoha, Kashiwa, Chiba, 277-8587, Japan
E-mail: nagai.yuki@jaea.go.jp

Abstract. We propose an experimental way to determine the pairing states for the unconventional superconductor Cu$_x$Bi$_2$Se$_3$. Using the spectral polynomial expansion method, we numerically calculate the local density of states (LDOS) in the multi-orbital tight-binding model and analytically obtain the zero-energy solution around a vortex. Both calculations reveal that a quantized vortex is spin-polarized for the gap function categorized by “pseudo scalar” which is the isotropic odd-parity order parameter. On the other hand, no clear spin-polarization around a vortex can observed for the gap function categorized by “polar vector” which breaks the rotational isotropy in the normal states.

1. Introduction
The topological insulators and superconductors have attracted much attention of theorists and experimentalists, because of their topologically protected nature of gapless surface states originated by non-trivial topology of the bulk wave function. So far, numerous works on topological insulators have been published [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11], while topological superconductors have been not much studied due to relatively little variety.

Cu-intercalated Bi$_2$Se$_3$ (Cu$_x$Bi$_2$Se$_3$), which is an electron-doped superconductor whose superconducting transition temperature $T_c \sim 0.3$K, has been regarded as a key compound to investigate the unconventional superconductivity with the non-trivial topology (topological superconductivity)[12, 13, 14, 15]. The mother compound Bi$_2$Se$_3$ is well-known as a 3-dimensional topological insulator by the non-trivial $Z_2$ topology. Recently, zero-bias conductance peaks (ZBCP’s) were observed using the point contact spectroscopy[16, 17], which are well-known as a signature of unconventional superconductivity such as $d$-wave, sign-reversing $s$-wave and $p$-wave Cooper pairs[18, 19, 20]. The observed ZBCP is generally caused by the Andreev bound states formed at surfaces or in vortex cores where the phase variation of the order parameters occurs. On the other hand, it is also known that the ZBCPs are observable owing to the topological origin in the chiral $p$-wave superconductor such as Sr$_2$RuO$_4$, and its topologically-protected gapless states are regarded as Majorana fermions[20]. Then, the ZBCP observed in Cu$_x$Bi$_2$Se$_3$ may be also a signature of a topological superconductivity. Therefore, it is important to obtain a clear evidence of the topological superconductivity.

In the superconductor, Cu$_x$Bi$_2$Se$_3$, Sasaki et al. theoretically demonstrated how the Majorana fermion brings about ZBCP’s [16]. Their theoretical calculations have revealed that the odd-parity spin-triplet pairing is the most-likely pairing to explain the observed ZBCP’s. However, they could not select only a possible pairing among four possible types of odd-parity pairing.
in Cu$_x$Bi$_2$Se$_3$, since the ZBCP can occur even in other pairing states responding to a variation of parameters in the original tight-binding model. Therefore, it is hard to identify the pairing symmetry only through ZBCP, i.e. the energy dependence of the density of states.

In this paper, we propose two methods to determine the pairing state in Cu$_x$Bi$_2$Se$_3$. In the first one, the strong anisotropic thermal conductivity can be employed as an evidence of the spin-polarized Cooper pairs referred as the gap function $\Delta_4$[25], one of four possible odd-parity parings. In the second one, the spin-polarized vortex-core bound-states can be done as that of the isotropic spin-triplet Cooper pairs referred as the gap function $\Delta_2$. Thus, there are two ways to distinguish between the gap function $\Delta_2$ and $\Delta_4$. We also discuss that some of the gap functions break the rotational isotropy in the normal states, regardless of the material parameters, in terms of the massive Dirac formulation. The structure of this paper is as follows. In Sec. 2, we discuss general properties of the tight-binding model Hamiltonian equivalent with the massive Dirac Hamiltonian which is a low-energy effective model and show that the gap function $\Delta_4$ usually has point-nodes. In Sec. 3, two theoretical treatments to examine a single vortex numerically and analytically are presented. Section 4 shows details of the numerical calculation results. In Sec. 5, it is demonstrated with the solution of the zero-energy and the spin-polarized vortex usually occurs for the gap function $\Delta_4$. Section 6 gives the conclusions.

2. General Background

An effective theory for the topological superconductor Cu$_x$Bi$_2$Se$_3$ can be described by the Nambu representation of the two-orbital model with spin-orbit coupling, whose form is expressed by the massive Dirac Hamiltonian[25]:

$$H = \int dr \left( \begin{pmatrix} \bar{\psi}(r) & \bar{\psi}_c(r) \end{pmatrix} \begin{pmatrix} \hat{H}^+_\text{eff}(r) & \Delta^-(r) \\ \Delta^+(r) & \hat{H}^-_\text{eff}(r) \end{pmatrix} \begin{pmatrix} \psi(r) \\ \psi_c(r) \end{pmatrix} \right),$$

where

$$\hat{H}^\pm_\text{eff}(r) = M(-i\nabla) + A_x(-i\nabla)\gamma^1 + A_y(-i\nabla)\gamma^2 + A_z(-i\nabla)\gamma^3 \pm \epsilon(-i\nabla)\gamma^0.$$  \hspace{1cm} (2)

Here, $\gamma^i$ is $4 \times 4$ Dirac gamma matrix. The gamma matrices in the Dirac representation is expressed as $\gamma^0 = \sigma_z \otimes 1$, $\gamma^i = 1 \otimes \sigma_i$, and $\gamma^5 = \sigma_x \otimes 1$ with $2 \times 2$ Pauli matrices $\sigma_i$ in the orbital space and $\sigma_i$ in the spin space, $\psi(r)$ is the Dirac spinor, $\psi(x) \equiv \psi^T(x)\gamma^0$, $\psi_c(x) \equiv \psi_c(x)\gamma^0$, and $\psi_c \equiv C\bar{\psi}^T$, where $C(\equiv i\gamma^2\gamma^0)$ is a representative matrix of charge-conjugation. The gap functions are defined as $\Delta^- \equiv \gamma^0\Delta_0\gamma^2$ and $\Delta^+ \equiv \gamma^0(\Delta^-)^\gamma_0$. $M$, $A_i$, and $\epsilon$ are the parameters depending on the material. It is noted that the order parameter $\Delta^-$ is determined by the on-site pairing interaction. According to Table I in Ref. [25], possible six gap functions are characterized by a pseudo-scalar, scalar, and polar vector (four-vector):

$$\Delta^- = \Delta_0, \Delta_0\gamma^5, \Delta_0\phi\gamma^5,$$  \hspace{1cm} (3)

where, $\Delta_0$ is a scalar parameter, the Feynman slash $\phi$ is defined by $\sum_{\mu}\gamma^\mu a_\mu$, and the gap function is characterized by the four-vector $a_\mu$. In the superconducting state, the gap functions represented by $a_\mu$ with finite $a_i$-components ($i = 1, 2, 3$) break the rotational symmetry and bring about the anisotropic electronic state, even if the normal state is isotropic. This induced anisotropy results in the angle-dependent thermal conductivity. Thus, the anisotropic thermal conductivity can be a clear evidence of the gap function represented by the four-vector $a_\mu$ [25].

Next, we discuss point-nodes of the gap function $\Delta_4$. Here, we define the gap function $\Delta_{4a}$ with the four-vector $a_\mu = (0, 0, 1, 0)$ ($\Delta_{4a}^+ = \Delta_{11}^a = -\Delta_{12}^a = -\Delta_{21}^a$). In this case, the gap function has the rotational symmetry around $y$-axis, and therefore the point-nodes can exist only on the $k_y$-axis (See, Fig. 1). In order to find the point-nodes, we must solve the above
Figure 1. Schematic figure of the polar vector for the gap function $\Delta_{4a}$.

Hamiltonian. The eigenvalues of the Hamiltonian can be obtained through the BdG equations described as

$$
\begin{pmatrix}
\gamma^0 \hat{H}_{\text{eff}}(r) & \gamma^0 \Delta-^{T}(r) \\
\gamma^0 \Delta^+^{T}(r) & \gamma^0 \hat{H}_{\text{eff}}^{*}(r)
\end{pmatrix}
\begin{pmatrix}
u(r) \\
u_{c}(r)
\end{pmatrix}
= E
\begin{pmatrix}
u(r) \\
u_{c}(r)
\end{pmatrix}.
$$

With the use of the relation $\lim_{k_{x} \to 0} A_{y}(k) = \lim_{k_{z} \to 0} A_{z}(k) = 0$ in this model, one can obtain the condition that the point-nodes exist:

$$A_{y}(k_{x} = 0, k_{y}, k_{z} = 0)^{2} = \Delta_{0}^{2} + \epsilon(k_{x} = 0, k_{y}, k_{z} = 0)^{2} - M(k_{x} = 0, k_{y}, k_{z} = 0)^{2}.
$$

In the normal state, the Fermi surface is determined by $\Delta_{0}^{2} = \sqrt{A(k)^{2} + M(k)^{2}} - \epsilon(k)$. Therefore, in the case of the small order-parameter $\Delta_{0} \ll M, \epsilon$, the point-nodes usually exist near the Fermi level. As the above discussion, the gap functions represented by a polar-vector such as $\Delta_{4a}$ can be identified experimentally in terms of the anisotropy of the physical quantities such as an angle-dependent thermal transport measurements[25]. One can conclude that the gap function is $\Delta_{4}$ if the thermal conductivity becomes anisotropic below $T_{c}$. On the other hand, we need to have another ways to determine the pairing function if the measured thermal conductivity is isotropic below $T_{c}$. Therefore, in this paper, we show that one can conclude that the gap function is $\Delta_{2}$ if spin-polarized vortices are observed.

3. Model and Method
In this section, we introduce the models for both of the numerical and analytical calculations to determine the gap function $\Delta_{2}$ represented as a pseudo-scalar.

In the numerical calculation, we use the mean-field tight-binding Hamiltonian in the Bogoliubov-de Gennes scheme,

$$
H = \sum_{k_{z}} \sum_{i,j} \begin{pmatrix} c_{i}^{\dagger} & c_{i}^{T} \end{pmatrix} \begin{pmatrix} H_{ij}(k_{z}) & \Delta f(R_{i}) \delta_{ij} \\
\Delta^{\dagger} f(R_{i})^{*} & -\hat{H}_{ij}^{*}(-k_{z}) \end{pmatrix} \begin{pmatrix} c_{j} \\
c_{j}^{*} \end{pmatrix},
$$

where $c_{i}^{\dagger}$ is the 4-component creation operator at the $i$-th site on the two-dimensional triangle lattice and $k_{z}$ denotes the momentum in the crystal $c$-axis. $\Delta$ is $4 \times 4$ matrix whose elements are given as $\Delta_{\alpha\alpha'}^{lm}$ with orbital $l(m)$ and spin $\sigma(\sigma')$ indices. The normal state matrix $\hat{H}_{ij}(k_{z})$ is given by

$$
\hat{H}_{ij}(k_{z}) = \int dR_{\perp} e^{ik_{z}(-R_{i} - R_{j})} \hat{H}(k_{\perp}, k_{z}),
$$
with \(ab\)-plane momentum \(k_\perp\). The \(4 \times 4\) matrix \(\hat{H}(k_\perp, k_z)\) is given as

\[
\hat{H}(k_\perp, k_z) = M(k_\perp, k_z) \gamma^0 + \gamma^0 A_x(k_\perp) \gamma^1 + \gamma^0 A_y(k_\perp) \gamma^2 + \gamma^0 A_z(k_\perp) \gamma^3 + \epsilon(k_\perp, k_z),
\]

where, \(M(k_\perp, k_z) \equiv M_0 - 2B_1(1 - \cos(k_z)) - B_2\eta(k_\perp)\), \(A_x(k_\perp) \equiv (2/3)A_2\sqrt{3} \sin(\sqrt{3}k_x/2) \cos(k_y/2)\), \(A_y(k_\perp) \equiv (2/3)A_2\cos(\sqrt{3}k_x/2) \sin(k_y/2) + \sin(k_y)\), \(A_z(k_\perp) \equiv A_1\sin(k_z)\), \(\epsilon(k_\perp, k_z) \equiv 2D_1(1 - \cos(k_z)) + D_2\eta(k_\perp) - \mu\), and \(\eta(k_\perp) \equiv (3 - 2\cos(\sqrt{3}k_x/2) \cos(k_y/2) - \cos(k_y))\).

We set \(M_0 = 0.28\) eV, \(A_1 = 0.32\) eV, \(A_2 = 4.1/a\) eV, \(B_1 = 0.216\) eV, \(B_2 = 56.6/a^2\) eV, \(D_1 = 0.024\) eV, \(D_2 = 19.6/a^2\) and \(a = 4.076\) Å as the material parameters for \(\text{Cu}_x\text{Bi}_2\text{Se}_3[16]\). For simplicity, we do not solve the gap-equation but use a spatial distribution form of the order parameter around a single vortex \(f(R_i)\) written as

\[
f(R_i) = e^{i\theta} \Delta_0 \frac{|R_i|}{\sqrt{|R_i|^2 + \xi^2}},
\]

where \(\theta\) denotes the polar angle around \(c\)-axis, \(\Delta_0\) is the amplitude of the order-parameter and \(\xi\) is the coherence length. We solve this \(8N \times 8N\) matrix BdG equations without self-consistent calculations. Here, \(N\) is the total number of lattice sites. To access large scale systems, we adopt the polynomial expansion scheme to calculate the local density of states (LDOS) \(n(\omega, i)[21, 22, 23]\). In this scheme with the Chebyshev polynomials, LDOS \(n(\omega, i)\) is expressed as

\[
n(\omega, i) \sim \frac{1}{\pi} \sum_{n=0}^{N-1} \frac{n! \cos(n \arccos(\bar{\omega}))}{\sqrt{1 - \omega^2}} \left(\frac{2}{n+1}\right) e^{(i)^T e_n(i)},
\]

where \(2N\)-component unit-vector \(e(i)\) is determined by \([e(i)]_\gamma = \delta_{i,\gamma}\) and \(e_n(i)\) is recursively generated by

\[
e_{n+1}(i) = 2\hat{K}e_n(i) - e_{n-1}(i), \quad (n > 1),
\]

\[
e_1(i) = \hat{K}e(i), \quad e_0(i) = e(i).
\]

Here, \(g_n^L = \sinh[n_\eta(1 - n/n_c)]/\sinh[n_\eta]\) is a coefficient in the Lorentz kernel[23, 24] and \(\bar{\omega} = (\omega - b)/a\) and \(\hat{K} = (\hat{H} - \hat{f})/a\) denotes renormalized energy and Hamiltonian matrix, respectively. \(n_c\) is a cut-off parameter, \(\eta\) denotes a smearing factor, and \(a\) and \(b\) are renormalization factors.

In the analytical calculation, we adopt the Dirac Hamiltonian which is the low-energy linearized model of the Hamiltonian (2):

\[
\hat{H}^\text{di}(r) = M_0 - i\partial_x \gamma^1 - i\partial_y \gamma^2 - i\partial_z \gamma^3 + \mu \gamma^0,
\]

with the renormalized axes \((x, y, z) \rightarrow (A_2x, A_2y, A_1z)\). In this case, the order-parameter is determined by \(\Delta^-(r) \rightarrow \Delta^-(f(r))\).

In the numerical and analytical calculations, we consider only a gap function \(\Delta_2 = \gamma^2 \gamma^0\), since this does not break the rotational symmetry so that the solution can be obtained analytically.

**4. Numerical Results**

We consider \(L_x \times L_y\) triangle lattice sites with the closed boundary. The single vortex is located at \((i_x, i_y) = (L_x/2, L_y/2)\). We adopt \(L_x = 96\) and \(L_y = 96\), where the matrix dimension size is 73728. To obtain the LDOS \(n(\omega, i)\), the 40 \(k_z\)-points meshes are considered. We consider the gap-amplitude \(\Delta_0 = 0.3\) eV and the chemical potential \(\mu = 0.4\) eV for convenience of calculation. We use \(a = 30\) eV, \(b = -\mu, \eta = 1 \times 10^{-3}\) eV and \(n_c = 8000\) as the parameters in the polynomial
expansion scheme. Without a vortex ($f(R_i) = \Delta_0$), the gap function $\hat{\Delta}_2$ is fully-gapped, and the spin-degeneracies of each orbitals are found as shown in Fig. 2. With a vortex, one can find the zero-energy bound states at a vortex core. We find two bound states in the $k_z$-resolved LDOS as shown in Fig. 3. One has the linear dispersion relation around the zero-energy. Other has the flat dispersion relation at the mid-gap energy ($E/\Delta_0 \sim 0.5$). We find that the zero-energy bound states consist of only up-spin quasiparticles and the mid-gap bound states consist of down-spin quasiparticles at a vortex core. This result means that the vortex for the gap function $\Delta_2$ is spin-polarized. Far from a vortex, the intensity of the down-spin components rises as shown in Fig. 4. Thus, the partial LDOS has the oscillating function along the radial axis. We can explain the origin of this spin-polarized vortex with the use of the following analytical calculation.
5. Analytical Results

In the case of the gap function $\hat{\Delta}_2 = \gamma^2 \gamma^0$, we can obtain two zero-energy solutions[27] expressed as

$$ u_1(r) = \frac{e^{-\int_0^r |f(r')|dr'}}{\sqrt{\lambda_1}} \begin{pmatrix} \sqrt{\mu + M_0 J_0(\bar{r})} & 0 \\ 0 & 0 \end{pmatrix}, \quad u_{c1}(r) = \frac{e^{-i\theta} \sqrt{\mu - M_0 J_1(\bar{r})}}{\sqrt{\lambda_1}} \begin{pmatrix} 0 & 0 \\ -i\sqrt{\mu + M_0 J_0(\bar{r})} & 0 \end{pmatrix}, $$

$$ u_1(r) = \frac{e^{-\int_0^r |f(r')|dr'}}{\sqrt{\lambda_1}} \begin{pmatrix} 0 & e^{i\theta} \sqrt{\mu + M_0 J_1(\bar{r})} \\ -i\sqrt{\mu - M_0 J_0(\bar{r})} & 0 \end{pmatrix}, \quad u_{c1}(r) = \frac{e^{-i\theta} \sqrt{\mu + M_0 J_1(\bar{r})}}{\sqrt{\lambda_1}} \begin{pmatrix} 0 & 0 \\ -e^{-i\theta} \sqrt{\mu + M_0 J_1(\bar{r})} & 0 \end{pmatrix}, $$

with

$$ \lambda_1 = 4\pi \int_0^{\infty} dr \left[ (\mu + M_0) J_0(\bar{r})^2 + (\mu - M_0) J_1(\bar{r})^2 \right] e^{-2\int_0^r |f(r')|dr'}, $$

$$ \lambda_2 = 4\pi \int_0^{\infty} dr \left[ (\mu - M_0) J_0(\bar{r})^2 + (\mu + M_0) J_1(\bar{r})^2 \right] e^{-2\int_0^r |f(r')|dr'}.$$

Assuming the solution $\psi(r)^T = c_1(u_1(r), u_{c1}(r)) + c_1(u_1(r), u_{c1}(r))$, the eigenvalue equations are written as

$$ \begin{pmatrix} 0 & ikz \\ -ikz & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_{c1} \end{pmatrix} = E \begin{pmatrix} c_1 \\ c_{c1} \end{pmatrix}, $$

with

$$ v \equiv \frac{2\pi}{\sqrt{\lambda_1 \lambda_2}} \int_0^{\infty} dr r e^{-2\int_0^r |f(r')|dr'} \sqrt{\mu^2 - M_0^2 (J_0(\bar{r})^2 - J_1(\bar{r})^2)}. $$
Therefore, the dispersion relations are given by

\[ E = \pm v k_z, \]

and the coefficients \((c_1, c_2) = (1, \pm i)/\sqrt{2}\) do not depend on \(k_z\). We define spin-resolved LDOS expressed as \(n_\uparrow(E = \pm v k_z, r) \equiv |\psi_\uparrow|^2 + |\psi_\downarrow|^2\) and \(n_\downarrow(E = \pm v k_z, r) \equiv |\psi_\downarrow|^2 + |\psi_\uparrow|^2\). The spin-resolved LDOS \(n_\uparrow\) and \(n_\downarrow\) are written as

\[
n_\uparrow(E = \pm v k_z, r) \equiv \left( \frac{\mu + M_0}{2\lambda_1} + \frac{\mu - M_0}{2\lambda_1} \right) J_0(r^2) e^{-2 \int_0^r J(r') dr'},
\]

\[
n_\downarrow(E = \pm v k_z, r) \equiv \left( \frac{\mu - M_0}{2\lambda_1} + \frac{\mu + M_0}{2\lambda_1} \right) J_1(r^2) e^{-2 \int_0^r J(r') dr'}.
\]

These equations show that \(n_\uparrow\) is localized around a vortex core, since the Bessel function \(J_1\) becomes zero at the origin \((J_1(0) = 0)\). The numerical results can be reproduced by the above equations.

Let us discuss the reason of the spin-polarization. Equations (14) and (15) mean that the angular momentum is a good quantum number, since the Bessel functions are the eigenstates of the angular momentum. The rotational symmetry does not break in a superconducting phase, since the gap function \(\Delta_2\) is a “pseudo-scalar” gap function. It should be noted that \(i\partial_x \gamma_1 + i\partial_y \gamma_2\) includes a raising and lowering operators \(\partial_x \pm i\partial_y\) in the normal-state Hamiltonian (13). Thus, the up-spin and down-spin components have the different angular momentum. If the zero-energy states exist, a certain components of the wave function is proportional to the Bessel function \(J_0(r^2)\), since the zero-angular momentum state is the lowest energy state in the eigenstates of the angular momentum. The component with the zero-angular momentum depends on the direction of the vortex. On the other hand, for the gap function \(\Delta_{4a}\), the angular momentum is not a good quantum number, since the polar-vector breaks the rotational symmetry around \(z\)-axis. Thus, the wave-functions of zero-energy bound states consist of the linear combination of the eigenstates of the angular momentum, and then the vortex is not spin-polarized for the gap function \(\Delta_{4a}\). We conclude that a vortex of the gap function \(\Delta_2\) is a spin-polarized vortex in the wide parameter range, as shown in the numerical and analytical calculations.

6. Conclusion

In conclusion, we proposed how to identify the pairing state for CuBi2Se3. We numerically and analytically calculated the LDOS with a single vortex for the gap function \(\Delta_2\) which has the isotropic odd-parity spin-triplet Cooper pairs. We adopted the tight-binding model for the numerical calculation and the massive Dirac model for the analytical calculation. In the numerical calculation, we found two bound states in the \(k_z\)-resolved LDOS as shown in Fig. 3. One has the linear dispersion relation around the zero-energy with the up-spin dominant quasiparticles. The other has the flat dispersion relation at the mid-gap energy \((E/\Delta_0 \sim 0.5)\) with the down-spin dominant quasiparticles. In the analytical calculation, we obtained two degenerated solutions at the zero-energy around a vortex core. The spin-resolved LDOS shows that there is a spin-polarized vortex for the gap function \(\Delta_2\). We showed that the solutions around a vortex for this gap function are the eigenstates of the angular momentum but that for the gap function \(\Delta_{4a}\) can not be the eigenstates of the angular momentum because of the order parameter represented by the polar-vector. According to the numerical and analytical calculations, we concluded that a vortex of the gap function \(\Delta_2\) is a spin-polarized vortex in the wide parameter range.

References